MST e NEWS

June 2011

INSIDE

Views of the Review

2011 Materials Capability Review

The 2011 Materials Capability Review was held the first week of June and was organized around the three primary themes of the Laboratory's materials strategy. Presentation and poster sessions were devoted to research on defects and interfaces, specifically nuclear energy and actinides; extreme environments in the form of radiation; and emergent phenomena as in materials for clean energy. It also included an overview and tour of LANSCE.

Clockwise from top left: Steve Wender, Cevdet Noyan, and John Ullmann discuss LANSCE nuclear physics and materials science; committee members front row from left, Barbara Jones, Gary Was (chair), Rachel Segalman; back row, from left, Ralph Nuzzo, Brian Wirth, John Bercaw, Thomas Brill, Adam Schwartz, Sarah Tolbert, and Cevdet Noyan; Ruifeng Zhang (T-3) and committee member Barbara Jones discuss atomistic modeling and experimental studies of the shock response of copper/niobium nanolayered composites; detail from the Wednesday evening dinner; dinner at the O Eating House Restaurant included a presentation on Fukushima reactor studies by D Division Leader DV Rao; MST Deputy Division Leader Dave Teter, MPA Deputy Division Leader David Watkins, and MPA Division Leader Toni Taylor compare notes during one of the poster sessions.

From Wendy's Desk

The cover shows activity at our Materials Capability Review. In last month's column, I explained why we do the review and our expectations for outcomes. Now, I can tell you some about results. This year's review was organized primarily around Energy Security programs. The theme areas were Materials in Radiation Environments, Materials for Nuclear Energy (actinides focus), and Materials for Clean Energy. There will be a formal report, and I'll extract information from that report to present at an ADEPS or MST All-Hands. What I can tell you here is from the verbal outbriefing.

The committee once again commended the high-quality science across the board. All of you who participated did a great job, thank you. The committee specifically admired Andy Nelson's (MST-7) presentation of novel and exacting thermophysical properties measurements on oxide nuclear fuels that is very well integrated with companion modeling work (and companion presentation by Chris Stanek). They also praised the poster presentations of David Korzekwa (MST-6) on casting modeling, David Dombrowski (MST-6) on LEU fuel fabrication, and Cindy Welch (MST-7) on electrodes for fuel cells.

'The committee once again commended the high-quality science across the board.'

Lunch with early-career staff took a last minute turn when the committee requested we invite two or three staff for each committee member rather than the one:one ratio that we had invited earlier. We scrambled to locate additional participants that day, and I am grateful to those of you who were able to join us on very short notice. The committee decided to split into groupings of two panelists with several staff, and they reported back that the format worked beautifully and that they got a lot of good input. In general, they heard about exciting and challenging work fostered by productive mentor/mentee relationships. They noted a gap in our process of transitioning from postdoc to staff scientist, in which the mentoring relationship is dropped abruptly. We will look into setting up a cross-organizational early-career mentoring program to address this gap (send me your ideas!).

Once again, the bureaucratic burden came into many discussions. This is supposed to be a scientific review and, as such, the committee is rightfully loath to attack such issues. Nonetheless, it has been a recurring theme and, therefore, they asked numerous insightful questions. They were encouraged to hear that we have turned a corner on doing science in the Plutonium Facility and the vector is upward, albeit with much progress yet to be accomplished, and also to hear that Director Anastasio, in his final month, established expectations that the new director and NNSA should be working to re-equilbrate the balance between safety processes and getting work done. The committee locked onto the need for "shared fate" across direct/indirect lines and a graded approach, so I believe its report will have tangible suggestions in these regards.

I do want to fit in an additional brief topic this month. Some of you may have met Solutions Teams from our Worker Safety and Security Team (WSST) coming through your labs, or you may be on one of these teams. The purpose is to use the peer relationship in a helpful manner to point out safety issues that might not be obvious to a person who works in a lab daily and to assist in addressing problems that you might be having difficulty getting fixed. These co-workers walking through your labs are not police, they do not report to me, and they find this activity valuable enough that they are volunteering time out of their busy schedules to perform the walkdowns. Each member serves a three-month rotation, so all of you will eventually have the opportunity to see the good practices and the problems we have in our labs and offices. Welcome these teams into your space, you'll be glad you did! They have my ear and my strong support for what they are doing, and they will only disclose your identity to me with your permission. If they need Division pull to get something done or funds (to a limited extent!), all they have to do is ask me. They are your advocates, and I see them making a positive difference already.

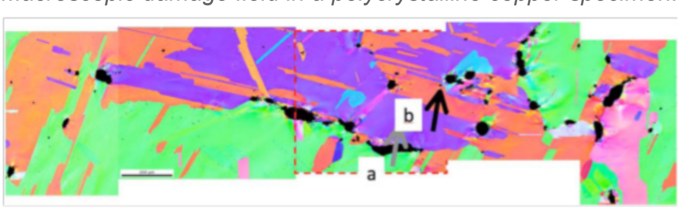
MST Division Leader Wendy Cieslak

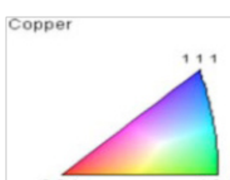
Small-scale experiments support materials strength and damage modeling

The limited understanding of the stochastic way in which polycrystalline materials deform, damage, and fail prevents accurate prediction of the material's performance. In an effort to enhance their ability to predict performance, Los Alamos researchers and collaborators are investigating dynamic damage evolution in bulk metals. Understanding how this process occurs could ultimately lead to the design of new, more failure-resistant materials.

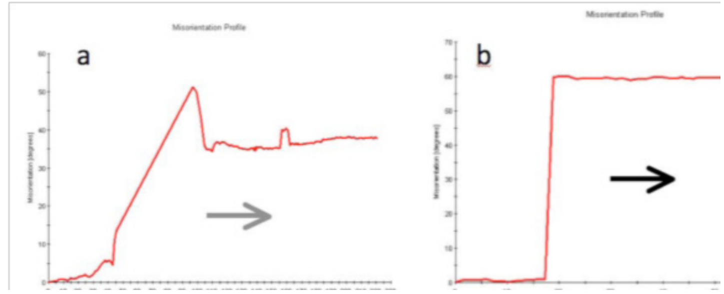
To understand the way in which damage evolves under dynamic loads, the researchers examined the coupling of loading profile to microstructural characteristics (see figures). The researchers observed that transitions between nucleation-dominated and growth-dominated damage evolution scale with grain size and/or defect density. The type of defect available may be critically important to the damage evolution, for example grain boundary type. The scientists examined misorientation across boundaries. Their analysis revealed that while generalized high angle boundaries are prone to damage nucleation, special boundaries are not. Special boundaries typically have lattice coincidence. These same boundaries can then be described by the number of coincidence lattice points shared by the grains on either side of the boundary. Generalized high angle boundaries are those that do not preserve lattice coincidence as well. Future work will focus on generalizing analysis to dynamic environments and microstructural defects to acquire a model for tailoring the failure response of structural metals.

Macroscopic damage field in a polycrystalline copper specimen.





Higher magnification view of a selected damage region in this same specimen (a) is the damaged boundary, and (B) in the undamaged boundary. Using these maps, misorientation across boundaries that were damaged and those that were not damaged can be traced. Misorientation is a way in which a boundary can be partially characterized.



Representative misorientation profiles for a damaged (a) and an undamaged (b) boundary.

Collaborators include Ellen Cerreta, Juan Pablo Escobedo-Diaz, Alejandro Perez-Bergquist, Carl Trujillo, Rusty Gray, Veronica Livescu, and Ricardo Lebensohn (Structure/Property Relations, MST-8); Brian Patterson (Polymers and Coatings, MST-7); Darcie Dennis-Koller (Shock and Detonation Physics, WX-9); Curt Bronkhorst, Irene Beyerlein and Ben Hansen (Fluid Dynamics and Solid Mechanics, T-3); Davis Tonks (Materials and Physical Data, XCP-5); and Fang Cao (ExxonMobil).

The Laboratory Directed Research and Development (LDRD) program, the DOE Energy Frontier Research Center for Materials at Irradiation and Mechanical Extremes (CMIME), and the Joint Department of Defense and Department of Energy Munitions Technology Development Program funded different aspects of the research. The work supports the Global Security and Nuclear Deterrence mission areas and the Materials for the Future and Information Science and Technology capability areas.

Technical contact: Ellen Cerreta

Multiscale study of the role of microstructure in the deformation behavior of hexagonal materials

Quantitative predictive models of the plastic response of metals are valuable tools for the design of parts and for improving forming processes. For example, understanding the formability of hexagonal close packed (HCP) materials such as magnesium, zirconium, titanium, and beryllium, which are used in automotive, nuclear, aeronautic and defense technologies; is extremely relevant for these applications and requires understanding deformation twinning, an important deformation mechanism in HCP materials.

Los Alamos scientists have developed a multiscale modeling paradigm that passes information from the microscale (atomistic)

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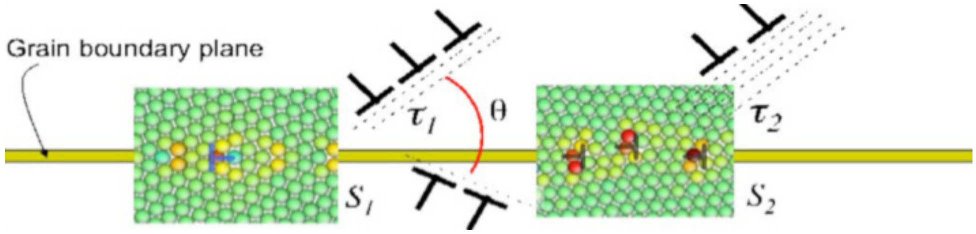


Schematic showing the statistical elements of the grain boundary model. Spatial distribution of grain boundary dislocation configurations, characterized by nucleation threshold stresses S_1, S_2 …. Space and strength distribution of stress states t_1, t_2…. associated with dislocation configurations at the boundary. Twin nucleation takes place when local stress exceeds local threshold stresses.

Multiscale . . . to the mesoscale (individual grains) and to the macroscale (polycrystalline metal). The multiscale model, which simulates hardening and texture evolution associated with plastic forming, includes a statistical treatment of twin nucleation at grain boundaries. The research reveals that twinning controls the characteristics of the macroscopic response observed in all the HCP materials studies.

Researchers include Carlos Tome and Jian Wang (MST-8), Rodney McCabe (Metallurgy, MST-6), and Irene Beyerlein (T-3). Reference: "A Multiscale Statistical Study of the Twinning of Magnesium," *Journal of the Minerals, Metals and Materials Society* **63** (3), 19 (2011). The DOE, Office of Basic Energy Sciences funded the research, which supports the Laboratory's Energy Security mission areas and the Materials for the Future and Information Science and Technology capabilities.

Technical contact: Carlos Tome

Fast Fourier transform-based modeling determines micromechanical fields in polycrystals

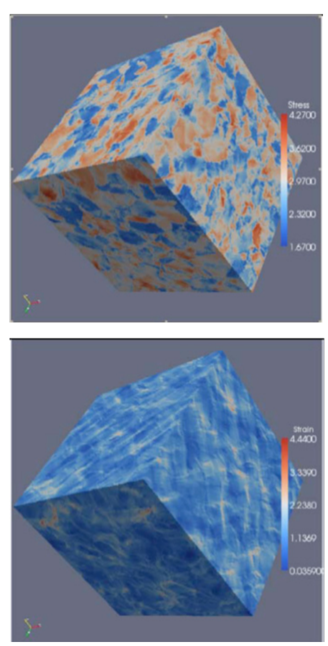
Emerging characterization methods in experimental mechanics of materials pose a challenge to modelers seeking to devise efficient formulations that enable interpretation and exploitation of the massive amount of data generated by these novel methods.

In an overview article in the *Journal of the Minerals, Metals and Materials Society,* Ricardo Lebensohn (MST-8), Anthony Rollett (Carnegie-Mellon University), and Pierre Suquet (Laboratoire de Mécanique et d'Acoustique/CNRS, France) report the use of a numerical formula based on fast Fourier transforms (FFT) applied to plastically-deforming polycrystalline materials. The FFT algorithm is a numerical tool extensively used in signal and image processing, which these scientists extended to solve a micromechanical problem. Their research shows that the FFT-based model can use voxelized microstructural images of heterogeneous materials as input. It is a viable alternative for performing micromechanical analyses of these large data sets. This efficient model can predict the mechanical response of a polycrystal directly based on a three-dimensional image of its microstructure. The viscoplastic approximation to crystal plasticity is a useful tool for solving problems involving plastically deforming polycrystals.

Polycrystalline materials play a key role as structural materials in vast sectors of the economy, such as energy, auto manufacturing, aerospace, and defense. The mechanical response of these materials depends on their microscopic properties, which are heterogeneous, as they in turn depend on the orientation of the constituent crystals. Three-dimensional characterization of the orientation and distribution of these crystals in a model allows for increased applications of these measurements.

Reference: "Fast Fourier Transform-based Modeling for the Determination of Micromechanical Fields in Polycrystals," *Journal of the Minerals, Metals and Materials Society* **63**, 3 (2011) . The Laboratory's Joint DoD/DOE Munitions Technology Program and the Advanced Simulation and Computing Physics and Engineering Models, Materials Project funded the Los Alamos portion of the work. This supports the Lab's Global Security, Nuclear Deterrence, and Energy Security mission areas and the Materials for the Future and Information Science and Technology capabilities.

Technical contact: Ricardo Lebensohn

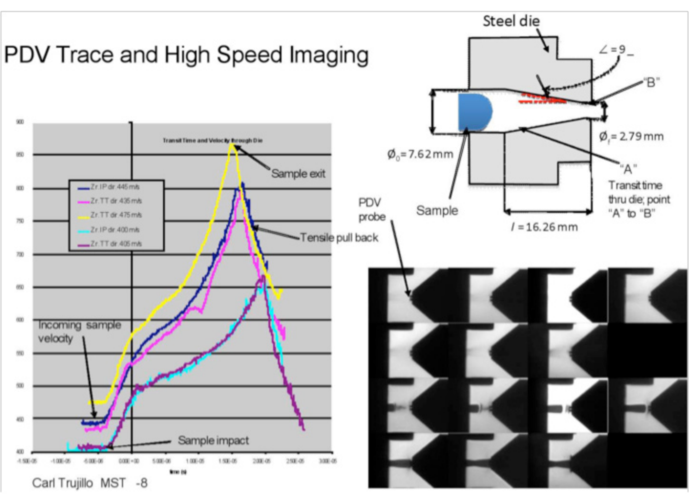


Von Mises equivalent stress and strain-rate fields predicted with the viscoplastic fast Fourier transforms (FFT)-based formulation, for an IN100 nickel alloy polycrystalline sample measured by serial-sectioning and orientation imaging microscopy.

Dynamic-tensile-extrusion of zirconium and the role of texture

The effect of high strain rate and high strains on mechanical behavior has been observed primarily in isotropic, cubic materials. The behavior of low-symmetry, textured, materials, however, is not as well understood.

To examine the high strain and high strain rate response of structural metals, Los Alamos researchers developed a dynamic extrusion technique in which high-purity zirconium bullets were accelerated up to velocities of 615 meters per second and extruded through a high-strength steel die. Scientists used the data to better understand material behavior at the microscale and by the modeling community to validate hydrocode constitutive models. A combination of in situ and ex situ characterization techniques examined the response of zirconium under this dynamic loading condition. In the experiment, a gas gun accelerated projectiles through a tapered constriction die in order to observe the dynamic extrusion profiles via high-speed imaging. An experimental measurement of transit time thru the die provided additional constraints on modeling approximations that allow the material to “slip” during the dynamic event in the die. Photonic Doppler velocimetry measured the sample velocity as it approaches the die and the velocity profile during the extrusion process (hence, transit time thru the die).



Top right): Schematic of the dynamic die extrusion experiment. (Left) Photonic Doppler velocimetry (PDV) results. IP is in plane zirconium specimens; TT is through thickness zirconium specimens. (Right) images from the experiment.

Researchers observed that in plane zirconium specimens developed larger elongations and more instabilities than through thickness zirconium specimens. Moreover, availability of slip systems in the in plane samples lead to deformation accommodated through slip and scattered twinning. Samples extruded along the through thickness direction first develop a more suitable microstructure by lattice reorientation prior to extensive slip. Participants include Carl Trujillo, Rusty Gray, Ellen Cerreta, Pablo Escobedo and Daniel Martinez (MST-8). The Joint Munitions Program (Eric Mas, LANL Program Manager) and Campaign 2 (Rick Martineau, LANL Program Manager) funded the research, which supports the Laboratory’s Global Security and Nuclear Deterrence mission areas and theMaterials for the Future capability. *Technical contact: Carl Trujillo*

Focus on materials for energy in this year’s Summer Lecture Series

The sixth annual Summer Lecture Series is underway and features talks by Laboratory scientists, tours of the Laboratory’s national user facilities, and closes out with an ice cream social. The series runs through July 27 with events held in a variety of locations.

MPA and MST divisions and the LANL Institutes sponsor the series, which presents a wide spectrum of LANL science to the Laboratory‘s students, postdoctoral researchers, staff, and visitors.

This year’s series includes 19 talks by distinguished LANL scientists and tours of the Los Alamos Neutron Science Center (June 24 and July 1), and the National High Magnetic Field Laboratory-Pulsed Field Facility (July 8). Lectures are open to LANL badge holders with selected lectures also open to the public. For schedule details, please see below. All talks and tours begin at 2 p.m.

Institutes Director Edward Kober (INST-OFF) said this year’s series theme is focused on materials for energy, which was motivated by recent events such as rising oil prices and the nuclear accident at Japan’s Fukushima Daiichi nuclear power plant.

“We try to expose the students to the broad range of science, missions, and applications that LANL is involved with,” Kober said. “Many people think of LANL as solely a nuclear weapons laboratory. We want to make sure that they become aware of the other half of our activities as well - and more generally, to just excite the students about careers in science and solving challenging problems.”

According to Kober, some of the most anticipated talks of the series are “Earthquake,” by Principal Associate Director for Science, Technology and Engineering Terry Wallace on June 22, and “Plutonium Nonproliferation” by former Laboratory director Siegfried Hecker on July 6.

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Series… "We thought the students would like to learn more about these (subjects) and it's an excellent chance to highlight LANL's expertise in those areas," Kober said.

For more information on the series, please see institutes.lanl.gov/institutes/docs/SLS_5-23-11.pdf or contact Debbie Wilke (INST-OFF). To sign up for tours contact Kelli Ingram (INST-OFF).

2011 Summer Lecture Series

Organized by MPA and MST Divisions and LANL Institutes

Our sixth edition of the Summer Lecture Series is designed to present the great science done at LANL to our students, postdoctoral researchers, staff and visitors. In the course of the talks and three site visits we will have a unique opportunity to see the facilities and learn about LANL directly from our top scientists. We look forward to meeting you there!

MAPS WITH LOCATIONS ARE SHOWN ON NEXT PAGES
All talks and tours start at 2:00PM.

DATE	LOCATION	AUTHOR AND TITLE
Wed. June 1	Rosen Aud.	Rajan Gupta: Emergent China and impacts of its development on the global energy and water resources
Fri. June 3	NHMFL	Chuck Mielke: National High Magnetic Field Tour
Mon . June 6	MSL Aud.	Alan Hurd: Energy Critical Elements
Wed. June 8	Study Center	Sriram Swaminarayan/Tim Germann: High Performance
Fri. June 10	CINT	Andrew Dattelbaum, Center for Integrated Nanotechnologies Tour
Mon. June 13	MSL Aud.	Dave Clark: Issues Surrounding Plutonium
Wed. June 15	Study Center	Gordon Jarvinen: Advanced Nuclear Energy Cycles
Fri. June 17	Rosen Aud.	David Dixon: Lessons from Fukushima
Mon. June 20	MSL Aud.	Blas Uberuaga: Radiation Damage in Nanomaterials
Wed. June 22	Study Center	Terry Wallace: Earthquakes
Fri. June 24	LANSCE	Alan Hurd: LANSCE Tour
Mon. June 27	MSL Aud.	Bette Korber: Vaccine design considerations for highly variable pathogens
Wed. June 29	Study Center	Ed MacKerrow: How People Become Terrorists
Fri. July 1	LANSCE	Alan Hurd: LANSCE Tour
Wed. July 6	Study Center	Sig Hecker: Plutonium Nonproliferation
Fri. July 8	NHMFL	Chuck Mielke: National High Magnetic Field Tour
Mon. July 11	MSL Aud.	Jennifer Hollingsworth: A bright future for solid-state lighting and quantum dots
Wed. July 13	Study Center	Dudley Herschbach: Barriers to Barrierless Reactions: Expect the Unexpected
Fri. July 15	Rosen Aud.	Steve Ashworth: Cool Power
Mon. July 18	Study Center	Albert Miligori: Science Challenges in Energy Storage
Wed. July 20	Study Center	Joe Martz: Plutonium Policy Issues
Fri. July 22	Rosen Aud.	Jim Smith: Experiments on liquid helium and superconductors
Mon. July 25	MSL	Roman Movshovich: Superconductivity: 100 year anniversary
Wed. July 27	MSL Courtyard Area	Ice Cream Social

For additional information please contact Debbie Wilke, dwilke@lanl.gov
To sign up for tours, please contact Kelli Ingram, kingram@lanl.gov

!!!Check LANL Institutes homepage frequently for program updates/changes!!!

Celebrating service

Congratulations to the following MST Division employees celebrating a service anniversary this month:

Stevan Patillo, MST-7	30 years
Sara Lucero, MST-7	15 years
Robert Hackenberg, MST-6	10 years

HeadsUP!

Personal electronic devices

Thumb drives, CD-R, DVD-R, and external drives are permitted on LANL property, however unclassified mandatory-protected information must be marked to identify the sensitivity level of the information (Unclassified Controlled Nuclear Information [UCNI], Personal Identifiable Information [PII], Naval Nuclear Propulsion Information [NNPI], and others), whether in a Limited Area, a Property Protection Area, or off-site.

Personal electronic devices (PEDs) in classified computing environments must be marked (as classified or unclassified) according to the highest classification and sensitivity level stored on the PED.

All PEDs introduced into a Laboratory Limited Area (for example, Sigma, BTF, and TFF) or above must be marked to identify ownership, for example, LANL, U.S. Government, or personal owner; as well as the information sensitivity level, where appropriate (For detailed information refer to policy P217).

To identify ownership, non-government owned devices may be marked as follows:

- A company property sticker
- A printed label with the owner's name
- An authorization form that identifies the device and device owner (Form 1897)

No PII, UCNI, or Official Use Only (OUO) information is allowed on thumb drives without encryption. The best way to ensure that you have the LANL preferred product is to ask your designated procurement representative (DPR) to purchase your thumb drive through iProcurement. Check with your OCSR for additional requirements for your particular area.

MST e NEWS

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To submit news items or for more information, contact Karen Kippen, EPS Communications, at 606-1822, or kkippen@lanl.gov.

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